Study of the Effects of the Antisite Related Defects in Silicon Dioxide of Metal-Oxide-Semiconductor Structure on the Gate Leakage Current

Ling-Feng Mao*, Zi-Ou Wang*, Ming-Zhen Xu, and Chang-Hua Tan****

Abstract—**The effects of the antisite related defects on the electronic structure of silica and the gate leakage current have been investigated using first-principles calculations. Energy levels related to the antisite defects in silicon dioxide have been introduced into the bandgap, which are nearly 2.0 eV from the top of the valence band. Combining with the electronic structures calculated from first-principles simulations, tunneling currents through the silica layer with antisite defects have been calculated. The tunneling current calculations show that the hole tunneling currents assisted by the antisite defects will be dominant at low oxide field whereas the electron direct tunneling current will be dominant at high oxide field. With increased thickness of the defect layer, the threshold point where the hole tunneling current assisted by antisite defects in silica is equal to the electron direct tunneling current extends to higher oxide field.**

Index Terms—**Silicon oxide, metal-oxide-semiconductor structures, tunneling**

I. INTRODUCTION

As lateral device dimensions has been scaled into the deep submicron regime to achieve high levels of speed and integration, there must be corresponding decreases in the gate oxide-equivalent thickness to maintain current levels required for circuit operation. Thus the gate leakage current exponentially increases with the oxide layer thickness decreasing, and it is necessary to precisely characterize the tunneling current through ultrathin oxide. On the other hand, the structure and formation mechanism of defects in crystalline and amorphous silica also plays an important role in the performance of microelectronics devices and fiber optics technology. As we know that a major concern in silicon technology is the reliability of complementary metal-oxide-semiconductor devices while they are scaled to smaller dimensions. Defect-mediated leakage and quantum-mechanical tunneling current are the main issue on the reliability of gate oxide. The point defects in silica will result in the localized states in the band gap of silica. They are potentially the sources of the gate leakage current. A large number of experimental and theoretical studies have been devoted to the characterization of the point defects in silica due to their role in the degradation of silica based electronic devices [1-12]. There are four categories of crystal defects in a crystal: point defects, line defects, area defects, and volume defects. Point defects include any foreign atom at a regular lattice site (i.e., substitutional site) or between lattice sites (i.e., interstitial site), antisite defects (e.g., Ga in As or As in Ga in compound semiconductors), missing lattice atoms, and host atoms located between lattice sites and adjacent to a vacant site (i.e., Frenkel defects). Antisite defects in the gate oxide (Si in O or O in Si) have not been thoroughly touched so far in the literature. Therefore the study of the effects of

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the antisite related defects in the gate oxide on the electronic conduction is necessary.

Stress induced leakage current can be regarded as a major dielectric reliability concern and have been extensively studied [13-18]. But the conduction mechanism for stress induced leakage current still remains an area of much discussion. For example: the neutral traps were believed to be the dominant cause of stress induced leakage current [17]; complex of a hydrogen atom with an oxygen vacancy was reported as the defect responsible for stress induced leakage current [18]. The hypothesis that neutral trap-assisted tunneling is a source of stress induced leakage current gains a wider acceptance. Combination of semi-emprical microscopic tight-binding calculations with full band Monte Carlo method was used to analyze defect-assisted elastic tunneling currents through ultrathin SiO_2 in metal-oxide-semiconductor field transistors in Ref. [19].

In the previous work [20], the effective mass issues in silicon nitride-oxide have been studied using the first-principles simulations. The relation between the concentration of nitrogen in lightly nitride silicon oxide and the tunneling current has been discussed on the basis of the first-principles simulations [21]. The effects of oxygen vacancy on hole tunneling current [22] and stress induced leakage current [23] have been studied by using first-principles simulations. The conduction band alignment of HfO_2 caused by oxygen vacancies and its effects on the gate leakage current in MOS structures have been studied by using first-principles simulations [24]. As we know antisite defects could be an origin of stress-induced leakage current. So it is necessary to study its effect on the tunneling current. The goal of the present paper is to build a picture of the effects of antisite defects on the electronic structure of SiO_2, and thus the increase in the tunneling current caused by antisite defects has been calculated using the results calculated from *ab initio* calculations.

II. METHOD

In this work, the band structures of alpha quartz supercells have been calculated using density functional theory in the local density approximation with the plane-wave pseudopotential method [25]. Amorphous silicon dioxide was believed to have similar band structure properties to those of alpha quartz, and the techniques used for determining the behavior of alpha quartz can also be applied to the more disordered structure of SiO_2 [26]. A supercell with eight α-quartz unit cells with or without one antisite defect is used to study the effect of the antisite related defects in the gate oxide on the gate leakage current in this paper.

The tunneling current are calculated according to the following equation [27]:

$$J = \int_0^\infty \frac{qm^*}{2\pi^2\hbar^3} D(E_x)\left(\int_{E_x}^\infty [f_r(E) - f_l(E)]dE \right) dE_x \quad (1)$$

where $D(E_x)$ is the transmission coefficient when the longitudinal electron energy is E_x. f_r and f_l are the distribution functions in the gate and the silicon substrate, m^* is the effective mass. The transmission coefficient $D(E_x)$ is calculated by a numerical solution to the one-dimensional Schrödinger equation. A parabolic $E(k)$ relation with an effective mass m^* as parameter is assumed in this work. The barrier is discretized by N partial subbarriers of rectangular shape covered the whole oxide layer. From the continuity of wave function and quantum current density at each boundary, the transmission coefficient is then found by:

$$D(E_x) = \frac{m_0}{m_{N+1}} \frac{k_{N+1}}{k_0} \frac{|\det M|}{|M_{22}|^2} \quad (2)$$

where M is a (2×2) product matrix, M_{22} is the quantity of the second row and the second column in this matrix $M = \prod_{l=0}^{N} M_l$ with the transfer matrices M_l given by:

$$M_l = \frac{1}{2} \begin{vmatrix} (1+S_l)\exp[-i(k_{l+1}-k_l)x_l] & (1-S_l)\exp[-i(k_{l+1}+k_l)x_l] \\ (1-S_l)\exp[+i(k_{l+1}-k_l)x_l] & (1+S_l)\exp[+i(k_{l+1}-k_l)x_l] \end{vmatrix} \quad (3)$$

In Eq.(3) $S_l = m_{l+1}k_l / m_l k_{l+1}$, and the effective masses and the momenta are discretized as $m_l = m^*[(x_{l-1}+x_l)/2]$ and $k_l = k[(x_{l-1}+x_l)/2]$, respectively, x_l is the position of lth boundary.

The entire oxide can be assumed to be composed of many supercells, (some with antisite defects and the others without). And thus dilute antisite defects can be calculated according to the following expression:

$$J = \frac{1}{S}\int_{s} j(x,y)ds \tag{4}$$

where S is the area of the oxide, j(x,y) is the local tunneling current. By using the Eq.4, the effects of the arbitrary the concentration of the antisite related to defects on the tunneling currents can be calculated. For simplicity, the defect oxide layer has been assumed to be composed of the same supercell and each supercell has one antisite defect in this work.

The Fermi-Dirac distribution has been used in the tunneling current calculations, and the maximum of the longitudinal electron (hole) energy has been set at 20 k_BT above (below) the conduction (valance) band, where k_B is Boltzmann constant, and T is the temperature. Two-step tunneling process has been used in the calculation of the defect-assisted hole tunneling current. The tunneling currents in this work have been calculated by using Eq. 1 according to two-step tunneling: the first step, from the gate (substrate) to the trap caused by the antisite related defects, the second step, from the trap to the substrate (gate).

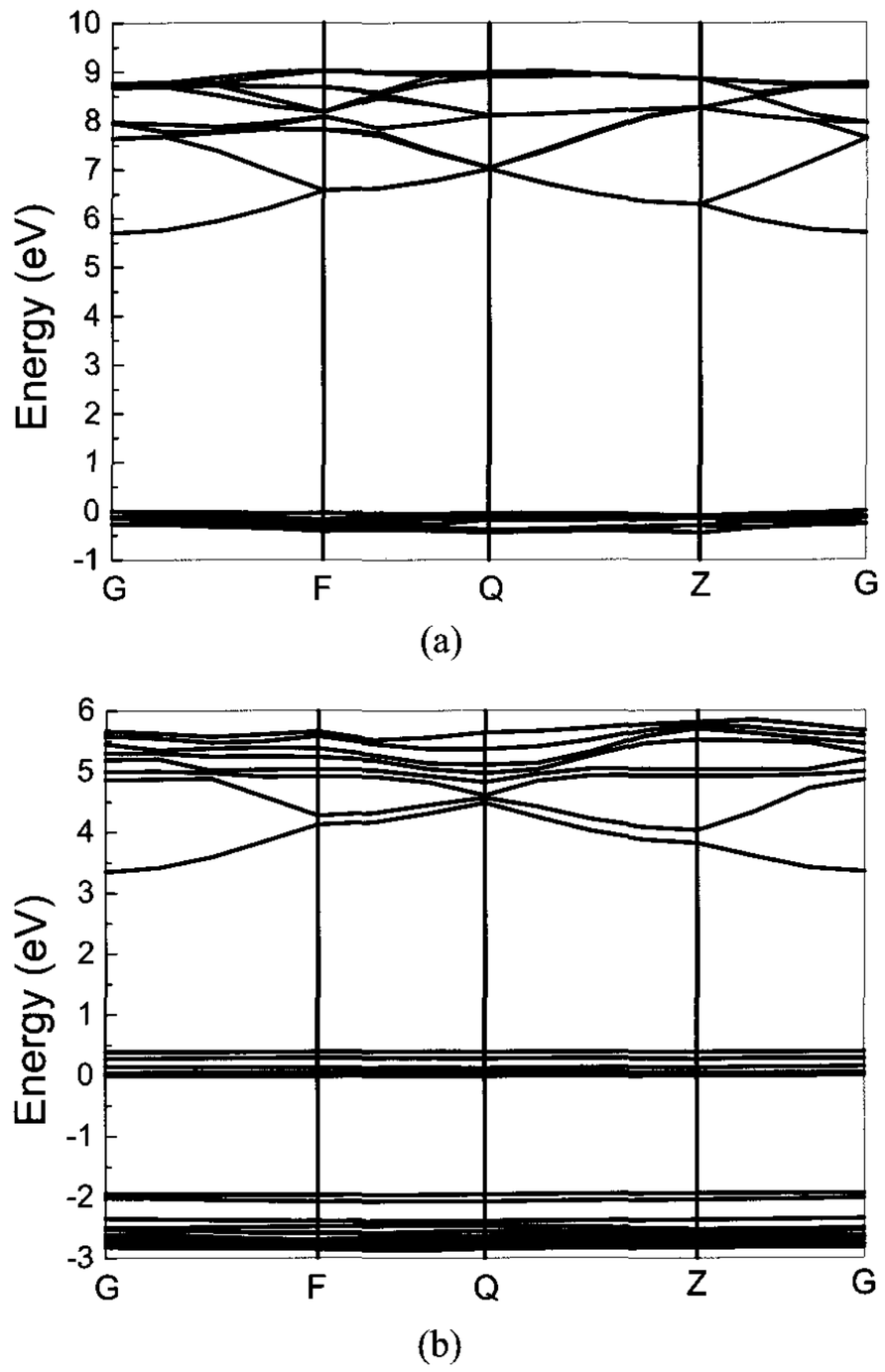

Fig. 1. (a) The band-structure diagram of the perfect SiO_2 supercell and (b) the defect SiO_2 supercell with the anti-sites defects.

III. Results and Discussion

The supercell with 72 atoms has been used to model defects in quartz [1] and to comparatively study the defect energetics in the monoclinic hafnium oxide and α-quartz [2]. The antisite related defect formation energy by using the supercell method in the first principles simulations has been obtained as 0.55 eV/atom in this work. As a comparison, the neutral oxygen vacancy formation energy is 6.2 eV/atom according to the total energy calculation in the first principles simulations, which is similar to the results obtained in Ref. [3]. It is obvious that the antisite defect formation needs less energy than that for the vacancy formation. It implies that the antisite related defects may be easily induced in the oxide because the oxygen vacancy have a larger formation energy. And oxygen vacancy has been regarded as a very important origin of stress-induced leakage current. Thus the discussion of the effects of antisite defects on the leakage current is necessary due to its lower formation energy.

Fig. 1(a), (b) shows the band structure of the perfect and defect alpha quartz supercell. Fig. 2 shows its density of states. Comparing Fig. 1(a) with Fig. 1(b), the energy levels above the valance band caused by the defects can be found to be in the bandgap of the alpha quartz supercell. The energy levels related to the antisite defect can be found within the band gap at 2.0 eV from the top of the valence band. Such localized states within the bandgap will assist holes tunneling through the oxide. It is also clearly seen in Fig. 2 that a large density of states due to the antisite related defects is found within the bandgap. Noted that there is a shift in Fig. 2 and Fig. 1(a), (b) because the reference energy is different in the first-principles calculations for both structures. Such a larger density of states means that local states can be introduced into the bandgap. And thus it can make a large contribution to the gate leakage current and may be an origin of the stress induced leakage current.

The tunneling currents have been calculated for an n-channel metal-oxide-semiconductor field transistor (n^+ poly gate, p substrate) in the mode of accumulation with negative gate voltage. The value of the bandgap of SiO_2 has been chosen as 8.6 eV, the electron barrier (hole)

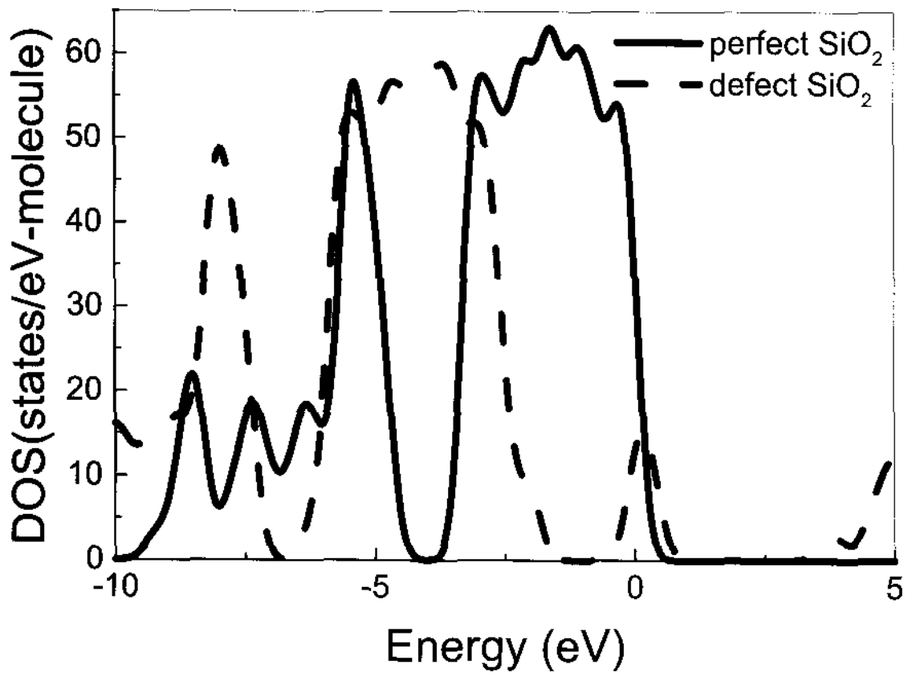

Fig. 2. The density of states the perfect SiO_2 supercell and the defect SiO_2 supercell with the anti-sites defects.

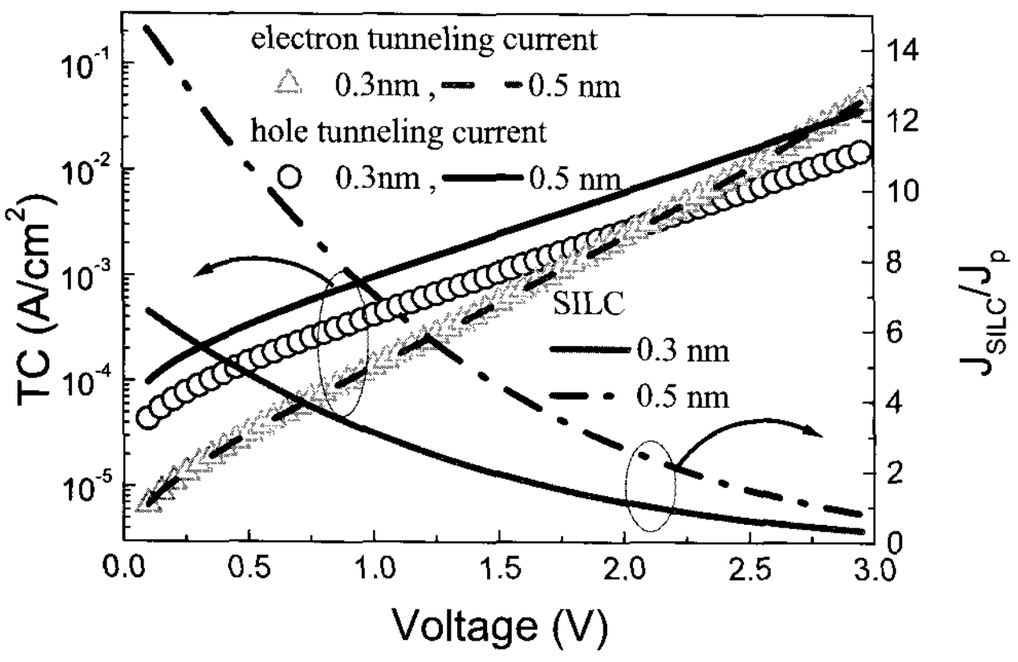

Fig. 3. Tunneling currents through 2 nm oxide when the defect layer locates at the SiO_2/gate interface and its thickness is 3 Å and 5 Å.

height has been chosen as 3.0 (4.5) eV, and the effective electron (hole) mass has been chosen as 0.5 (0.38) m_0 according to Ref. [28]. And these parameters have been used in the tunneling current calculations. And in the tunneling current calculations, the bandgap of SiO_2 has been assumed to be not affected by the antisite related defects. In the following, J_p is the tunneling current through the perfect oxide, and J_{SILC} is the stress induced leakage currents caused by the antisite related defects.

Fig. 3 shows that calculated tunneling currents through the oxide (its thickness is 2.0 nm) in an *n*-channel metal-oxide-semiconductor field transistor when the defect layer is located at the SiO_2/gate interface and its thickness is 3 Å and 5 Å. It is clearly seen in these figures that the hole tunneling current assisted by the antisite related defect will be dominant at the low oxide electric field and the electron tunneling current will be

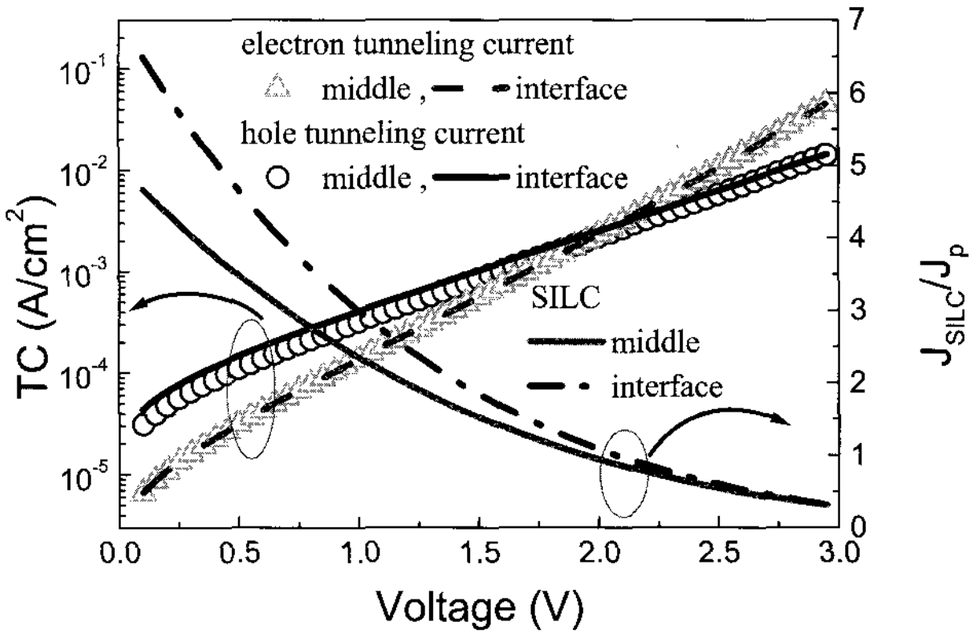

Fig. 4. Tunneling currents through 2 nm oxide when the defect layer with thickness being 3 Å locates at the middle of the SiO_2 layer and the SiO_2/Si substrate interface.

dominant at high oxide electric field. With increased thickness of defect layer that has the antisite related defects, the threshold point where the hole tunneling current assisted by the antisite related defects is equal to the electron direct tunneling current extends to higher oxide electric field.

Fig. 4 shows that calculated tunneling currents through the oxide in an *n*-channel metal-oxide-semiconductor field transistor with the oxide thickness as 2.0 nm when the defect layer is located at the middle of the oxide or at the SiO_2/Si substrate interface. It is also clearly seen from these figures that the hole tunneling current assisted by the antisite defects will be dominant at the low oxide electric field and electron-tunneling current will be dominant at high oxide electric field. Checking Fig. 3 and Fig. 4, the effects of the position of the defect layer on the leakage current can also be observed. When the defect layer located at the SiO_2/gate interface, the contribution of the hole tunneling current assisted by the antisite related defects to the leakage current is the largest, whereas the contribution of the hole tunneling current assisted by the antisite related defects to the leakage current is the smallest when the defect layer located at the middle of the oxide. It is well known that trap assisted tunneling can be described by two-step tunneling: the first step, from the gate (substrate) to the trap caused by the antisite related defects, the second step, from the trap to the substrate (gate). One can note that the tunneling probability of both from the gate (substrate) to traps and from the traps to substrate (gate) depends on the trap location. It is the reason why the position of the defect layer affects on the leakage current.

IV. SUMMARY

Based on the first-principles calculations, the antisite defect formation energy is obtained as 0.55 eV/atom by using supercell method in the first principles simulations. The antisite formation needs much less energy than vacancy formation does (the vacancy formation energy being 6.2 eV/atom). And the levels related to antisite related defects can be obtained within the bandgap at 2.0 eV from the top of the valence band.

Combining with the band structures obtained from first-principles simulations, tunneling currents through an ultrathin SiO_2 layer with the antisite related defects have been calculated. It is concluded that the hole tunneling current will be dominant at the low field and electron tunneling current will be dominant at high field. With increasing thickness of the antisite defects layer, the effects of hole tunneling current on leakage current extend to higher field. Stress induced leakage current may be origin from the formation of the antisite related defects. And the stress induced leakage current caused by antisite defects will be largest when the defect locates at the interface.

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REFERENCES

[1] C. J. Pickard, and F. Mauri, *Phys. Rev. Lett.* 88, 086403(2002).

[2] W. L. Scopel, A. J. R. da Silva, W. Orellana, and A. Fazzio, *Appl. Phys. Lett.* 84, 1492-1494(2004).

[3] S, Mukhopadhyay, P. V. Sushko, A. M. Stoneham, and A. L. Shluger, *Phys. Rev. B* 71, 235204(2005).

[4] Y. K. Kim, H. S. Lee, H. W. Yeom, D. Y. Ryoo, S.-B. Huh, and J.-G. Lee, *Phys. Rev. B* 70, 165320(2004).

[5] G. Buscarino, S. Agnello, and F. M. Gelardi, *Phys. Rev. Lett.* 94, 125501(2005).

[6] A. Yokozawa, and Y. Miyamoto, *Appl. Phys. lett.* 73, 1122-1124(1998).

[7] V. B. Sulimov, P. V. Sushko, A. H. Edwards, A. L. Shluger, and A. M. Stoneham, *Phys Rev. B.* 66, 024108 (2002).

[8] S. Agnello, R. Boscaino, M. Cannas, F. M. Gelardi, M. Leone, and B. Boizot, *Phys Rev. B.* 67, 033202 (2003).

[9] D. J. Chadi, *Appl. Phys. lett.* 83, 437-439(2003).

[10] A. S. Mysovsky, P. V. Sushko, S. Mukhopadhyay, A. H. Edwards, and A. L. Shluger, *Phys Rev. B.* 69, 085202 (2004).

[11] L. Skuja, *J. Non-Cryst. Solids* 236, 16-48(1998).

[12] P. E. Blöchl, *Phys Rev. B.* 62, 6158-6179(2000).

[13] M. Fadlallah, G. Ghibaudo, M. Bidaud, O. Simonetti, and F. Guyader, *Microelectronic Engineering*, 72, 241- 246 (2004).

[14] C. Petit, A. Meinertzhagen, D. Zander, O. Simonetti, M. Fadlallah, and T. Maurel, *Microelectronics Reliability*, 45, 479-485 (2005).

[15] D. Bauza, F. Rahmoune, R. Laqli, and G. Ghibaudo, *Microelectronics Reliability*, 45, 849-852(2005).

[16] A. Meinertzhagen, C. Petit, D. Zander, O. Simonetti, T. Maurel, and M. Jourdain, *J. App. Phys.*, 91, 2123-2132(2002).

[17] D. J. DiMaria, and E. Cartier, *J. App. Phys.*, 78, 3883-3894 (1995).

[18] P.E. Blöchl, and J.H. Stathis, *Phys. Rev. Lett.*, 83, 372-375 (1999).

[19] M. Städele, B. Fischer, B. R. Tuttle, and K. Hess, *Solid State Electronics*, 46, 1027-1032 (2002).

[20] L. F. Mao, Z. O. Wang, J. Y. Wang, and G. Y. Yang, *Semicond. Sci. Technol.*, 20, 1078-1082 (2005).

[21] L. F. Mao, and Ziou Wang, *Physica Status Solidi (a)*, 204, 784-790 (2007).

[22] L. F. Mao, *Microelectronics Reliability*, 47, 1213-1217(2007).

[23] L. F. Mao, *International Journal of Electronics*, 94, 985-99 (2007).

[24] L.F. Mao, Z.O. Wang, J.Y. Wang, and C.Y. Zhu, *Eur. Phys. J. Appl. Phys.* 40, 59-63 (2007).

[25] M. D. Segall, Philop J. D. Lindan, M. J. Probert, C. .J Pickard, P. J. Hasnip, S. J. Clark, and M. C. Payne, *J. Phys.: Condens. Matter.*, 14, 2717-2744 (2002).

[26] J. F. Verwey, E. A. Amerasekera, and J. Bisschop, *Rep. Prog. Phys.* 53, 1297-1331(1990).

[27] Y. Ando, and T. Itoh, *J. Appl. Phys*. 61, 1497-1502 (1987).
[28] M. I. Vexler, S. E. Tyaginov, and A. F. Shulekin, *J. Phys.: Condens. Matter* 17, 8057-8068 (2005).

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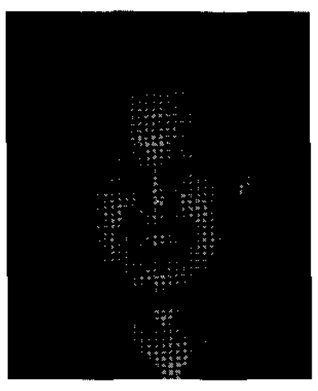

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